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Alexander M. Cruickshank and John H. Pere	epezko	
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The 1991 Gordon Research Conference on Physical the Plymouth College South location in Plymo Foundations of Microstructure Development. The alloys is a cornerstone of physical metallurgy thermodynamic and kinetic constraints, new microstructures may be possible. The discurdevelopments in such keynote issues as alloy diffusion in ordered alloys and multicomponent sy kinetics. There was a balanced coverage between experimental work involving verification tests and in the areas of aluminum alloys, aerospace mat program.	phase stability, crys ystems, interfacial structure een theoretical and d applications. In add	stal growth and solidification, acture and phase decomposition modeling analysis and critical dition, an industrial perspective
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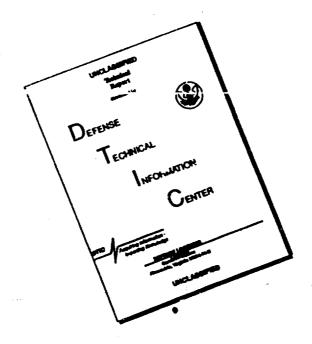
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#### FINAL REPORT

AFOSR Grant (AFOSR-91-0173) for the Support of the 1991 Gordon Conference on Physical Metallurgy

"Foundations of Microstructure Development"

#### Submitted to

Air Force Office of Scientific Research Division of Research Grants, Building 410 Bolling AFB, Washington, DC 20332-6448

Attention: Dr. Alan H. Rosenstein

#### Submitted by

Dr. John H. Perepezko (Co-Chairman and P.I.)
Professor, Department of Materials Science and Engineering
University of Wisconsin-Madison
1509 University Avenue
Madison, WI 53706

Dr. William J. Boettinger
National Institute of Standards and Technology
Metallurgy Division
Building 223 Room A153

#### and

Dr. Alexander M. Cruickshank (Director)
Gordon Research Conferences
University of Rhode Island
Kingston, RI 02881

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#### Introduction

The 1991 Gordon Research Conference on Physical Metallurgy was held July 29-August 2, 1991 at the Plymouth College South location in Plymouth, New Hampshire. The Conference topic was Foundations of Microstructure Development. US Government grants were made to the Gordon Research Conference to offset partially the travel and registration cost of many the speakers and discussion leaders, a few attendes, and the co-chairman. Grants totaled \$18,000.00. Of this total, \$6,000.00 each was provided by AFO3R (AFOSR-91-0173), ONR and NSF (DMR-9102779). In this final report a brief description of the conference is given and includes some of the highlights of the meeting and discussions.

#### Conference Description

The study of microstructural development in metals and alloys is a cornerstone of physical metallurgy. An effective approach to this theme can be developed by examining the limiting bounds for a given microstructural type. From an understanding of the compositional, thermodynamic and kinetic constraints, new levels of control and the development of new microstructures may be possible. As a result, the conference program was focused on the critical processes governing microstructural development. The discussion was organized to present state-of-the art developments in such keynote issues as alloy phase stability, crystal growth and solidification, diffusion in ordered alloys and multicomponent systems, interfacial structure and phase

decomposition kinetics. There was a balanced coverage between theoretical and modeling analysis and critical experimental work involving verification tests and applications.

The conference program was organized on the basis of the realization that major advances in physical metallurgy leading to novel insight or new discoveries have often occurred as a result of a steady, concerted study effort on an experimental and theoretical front to examine fundamental physical processes. Often the discoveries appear as anomalies, but with further examination the anomaly becomes recognized as a new aspect of a basic mechanism. In addition, there is an important realization that much of the work in the physical metallurgy of advanced materials is intended for eventual applications. As a result, the initial session of the first day provided that perspective in the areas of aluminum alloys, aerospace materials, and electronic materials. This was followed by a session on interface reactions where the theoretical and experimental developments including the latest studies were described. Since most metals undergo a melting and solidification process sometime during their fabrication, the importance of crystal growth and solidification is apparent and occupied most of the discussion of the second Similarly, the basis of materials processing is rooted in diffusional transformations which was the basic theme of the third day where the discussion ranged from the very early stages of precipitation to multicomponent systems and basic mechanisms of diffusion in more complex systems. This discussion carried over to the fourth day with some of the detailed studies of interface structure including the effects of elastic stresses. Finally, the program ended with discussion of ordering reactions and displacive transformation that are becoming recognized as crucial in many of the latest developments in transformation kinetics.

While every effort was made to identify frontier issues with each of the foundation topics, it was recognized that such a listing can not be completely comprehensive and still allow time for the extensive discussion that is the hallmark of a successful Gordon Conference. Certainly, further issues and perspectives were brought out in the discussion. However, each of the foundation topics could be a theme of a separate conference. Indeed one of the advantageous of the Gordon Conference forum is the ability to bring together various groups and perspectives to have a high level exchange of experimental and theoretical developments.

Following the tradition of previous Gordon Conferences, a relatively small number of speakers were invited to make presentations to the conference. The main purpose of these talks was to describe recent progress and set the stage for further thought and discussion. A copy of the program and speakers and discussion leaders is appended to this report. In addition, a poster session was also held during the conference in order to allow some of the participants to present their research results. This was a well attended session with over 20 contributed

posters, provided a basis for broad exposure of very new results and stimulated a great deal of excitement that are often continued late into the evening.

The conference attracted participants from a wide variety of institutions and backgrounds. A list of attendees appended to this report shows that a total of 124 scientists and engineers participated in the conference. Of these only 31 were on the program as speakers and discussion leaders. The attendees included 106 from the United States and 18 from foreign countries. Of these 68 were from universities, 37 from government laboratories or offices and 19 from industry. Finally it is worth noting that the number of applicants for this conference exceeded the number of places available.

#### Program Highlights

The major attraction at Gordon Conferences is the opportunity to interact on an informal level with a large number of scientists interested and knowledgeable in a given subject. Facilities at the Plymouth College catered to this aspect in a number of ways; the main lounge, the game room, and the grounds were excellent sites for informal discussion. These facilities were in use throughout the day and night for numerous small group discussions which led to the development of research ideas and interactions. This informal aspect of the Gordon Conference, was therefore a success.

In the formal program the initial session provided an industrial perspective on advanced materials. For example, Staley from Alcoa discussed aluminum alloy development and as

requested raised a number of issues for future work including how the grain size is limited by a various particles in aluminum alloys, some new areas in presolidification processing to initiate particulate formation, and the need for additives in aluminum alloys to remove undesirable impurities. In a similar vein Blackburn from Pratt & Whitney discussed the importance of modeling in scaling-up processing from laboratory operations to production operations. He also pointed out that the best property in any given category cannot usually be obtained in the best combination of properties and as a result process models are essential to allow for an optimum balance of properties. Rosenberg from IBM provided information on many exciting developments in the miniaturization of electronic circuits down to 0.1 microns in scale. Devices have been made in the laboratory, but again the point was made on how to scale-up the processing. He pointed out that more than 98% of system failures are related to metallization treatments and that this issue provides a wealth of important problems to deal with. Next, John Cahn provided an informative discussion of heterogeneous nucleation along the lines of Gibbs including very interesting new developments in wetting behavior and crystal morphologies. This discussion was complemented very nicely by Dahmen who provided some outstanding TEM micrographs to illustrate the development of crystal morphology at the atomic scale. day was devoted to solidification. Trivedi gave an overview of some of the unsolved problems in solidification microstructure development. He also provided useful insight into the understanding of study state processes and the development of microstructure over a range of velocity. Brown followed this with a more focused discussion on wavelength selection during cellular solidification where the complete domain of velocity-wavelength behavior is being mapped out including the important onset ranges of breakdown of planar interface and the various time scales appropriate for the different breakdown behavior. Dantzig gave summary of the modeling approaches to process development ranging from nucleation kinetics models, which are sorely lacking to approaches for accounting for growth kinetics and heat evolution during solidification. The evening session belonged to the theoreticans. Sekerka provided very effective introduction to the main theoretical developments in diffuse interface theories of crystal growth and phase field calculations of solidification. These are two approaches to deal the difficulties of matching solutions in the liquid and solid state at the interface. In the diffuse interface model Oxtoby described perturbation approaches where the liquid is treated as a perturbed solid and the solid treated as a perturbed liquid as a means of modeling their behavior. Wheeler approached the problem from phase field model method which deals with the existence of various potentials which are expressed in terms of an order parameter. While each approach has advantages, it is not clear at present which is superior. They both appear to give effective descriptions of observed behavior. Clearly more development of analysis is needed. On the third day Cohen provided an excellent overview of the early stages of

participation including the formation of GP zones, initially ordered configurations and clustering effects where strain energy factors become important. This is followed Purdy's discussion of precipitation in ternary systems where the concept of local equilibrium sometimes needs to be modified to include paraequilibrium i.e. equilibrium with respect to one component. The morning ended with a discussion by Greer of recent developments in solid state amorphization during interdiffusion reactions. The various thermodynamic and kinetic behaviors were analyzed including how to treat diffusion in the very steep concentration gradients that develop in multilayer structures at the onset of interdiffusion which is a new realization.

These discussions were followed in the evening by a presentation on diffusion in ordered alloys by Bakker who pointed out that there is a much stronger correlation factor in ordered crystals than in disordered crystals and that one must consider defect structures on the sublattices in ordered crystals. example, when this is done in Ni3Al, it is found that nickel can diffuse on its own sublattice at much the same rate as for self diffusion in pure nickel. Van Loo presented an elegant discussion of the Kirkendall effect during multiphase diffusion. He described methods to analyze diffusion path sequences in multicomponent systems which is crucial in the development of The importance of interfaces and domain composite structures. structures that develop in elastically strained systems was the high ight in the next session. Howe presented video images of lattice resolution TEM studies conducted at high temperature to

reveal the dynamics of interface motion. This is truly a remarkable experimental achievement. Voorhees discussed an interesting analysis of the competition between strain energy and interfacial energy in determining the equilibrium shape of a precipitate in the later stages of reaction. Roytburd followed with a detailed analysis of the formation and development of polydomain structures that often occur in twinning and martensite reactions and involve multiple subdivision with the development of increasing levels of elastic strain. The last two sessions dealt with various aspects of the thermodynamics and kinetics of ordering reactions. Inden gave an informative overview of phase diagram modeling starting from the regular solution all the way up to cluster variation methods that are used to treat more complex interactions. This is followed by Allen's analysis of the behavior of diffuse interfaces with respect to order parameter as well as concentration gradients. He applied this analysis to explain some of the domain coarsening kinetics observed in ordered alloy. In a detailed study of the kinetics of ordering reactions, Banerjee highlighted some of the crystallographic aspects. Often BCC phases transformations by various shears of (110) planes. In the last presentation Johnson tried to integrate the diffusive and displacive characteristics of transformations. It is becoming clear that both aspects can occur in given transformation types and that the traditional distinction between displacive and diffusional transformations is not as sharp as it has been viewed previously. As a sign of the interest and animated discussion during the conference, it is useful to point out that more than 85 people were on hand to hear the last presentation on Friday morning.

In light of the vigorous discussion, the foundations of microstructural development clearly generated a keen interest. Several emerging new issues in alloy phase stability, in crystal growth and solidification, diffusional reactions, interfacial structure and phase decomposition were highlighted during the meeting. Equally important is the industrial perspective that allowed for the often pointed out gap between theoretical and experimental developments and industrial applications to be bridged to some extent. New perspectives and new interactions were developed at the meeting which will yield future dividends.

#### Physical Metallurgy Gordon Conference Plymouth State Coilege (South), Plymouth, NH July 29 - August 2, 1991

William J. Boettinger and John H. Perepezko, Cochairmen Anthony W. Thompson and Robert O. Ritchie, Vice-Cochairmen

> 1991 Conference Topic Foundations of Microstructure Development

Morning sessions start at 3:30 AM Evening sessions start at 7:30 PM

Monday AM: Industrial Perspective on Advanced Materials (Alan Rosenstein, AFOSR)

James Staley, Alcoa

Martin Blackburn, Pratt & Whitney

Robert Rosenberg, IBM

Al Alloy Development

Advanced Aerospace Allovs

Electronic Materials

Monday PM: Interface Reactions (Frans Spaepen, Harvard)

John Cahn, NIST

Hetrogeneous Nucleation

Ulrich Dahmen, Lawrence Berkerley Lab. TEM Study of the Development of Grain

Boundaries & Precipitates

Tuesday AM: Solidification Microstructures (John Hunt, U. of Oxford)

Rohit Trivedi, Iowa State U.

Solidification Microstructures

Robert Brown, MIT

Nonlinear Dynamics & Wavelength Selection

in Cellular Solidification

Jonathan Dantzig, U. of Illinois-Urbanna

Macro/Micromodelling of Eutectic

Castings

Tuesday PM: Crystal Growth Kinetics (Bob Sekerka, Carnegie-Mellon)

David Oxtoby, U. of Chicago

Adam Wheeler, U. of Bristol

Diffuse Interface Theories of Crystal Growth

Phase Field Calculations of Binary Alloy

Solidification

Wednesday AM: Diffusional Transformations (Bill Morris, UC-Berkeley)

Jerry Cohen, Northwestern U.

Gary Purdy, McMaster U.

Lindsay Greer, U. of Cambridge

Early Stages of Precipitation

Precipitation in Ternary Systems

Solid-State Amorphization

Wednesday PM: Diffusion Mechanisms (John Morral, U. Conn.)

Hans Bakker, U. Amsterdam

Frans van Loo, Eindhoven U.

Diffusion Mechanisms in Ordered Intermetallics

Kirkendall Effect in Multiphase Diffusion

#### Thursday AM: Interfaces & Domains (Carol Handwerker, NIST)

Jim Howe, U. of Virginia

Peter Voorhees, Northwestern U.

Alexander Roytburd, U. of Maryland

HRTEM of Interfaces

Dynamics of Interfaces in Elastically Stressed

Solids

Formation of Polydomain Structures

Thursday PM: Ordering Transformations (Ben Burton, NIST)

Gerhard Inden, Max Planck Inst.

Eisenforschung

Sam Allen, MIT

Phase diagram Modeling

Diffuse Interfaces in Ordering Systems

Friday AM: Displacive Transformations (Lee Tanner, Lawrence Livermore)

Srikumar Banerjee, Bhabha Atomic Research Centre, Bombay, India

Bill Johnson, Carnegie-Mellon

Replacive/Displacive Ordering

Transformations Displaying Diffusive and Displacive Characteristics

### GORDON RESEARCH CONFERENCE Physical Metallurgy

## Registration List July 29 - August 2, 1991 Plymouth State College, Plymouth, NH

Dr. Ralph Adler Army Materials Tech. Lab. SLCMT-EMM Arsenal St. Watertown, MA 02172	625	Dr. Michael Baskes US Dept. of Energy Division of Material Sciences ER Washington, DC 20585	404 -131/GTN
Dr. Robert Aikin Jr. Martin Marietta Labs. 1450 South Rolling Rd. Baltimore, MD 21227	719	Paxal Bellon SRMP, Centre D/Etudes de Saday Elsur Yrette, France 91191	606
		Dr. Leonid Bendersky	304
Dr. Donald Robert Allen University of Wisconsin Dept. of Materials Sci. & Engineer:	511 ing	NIST, Metallurgy Div. BLDG 223,A Gaithersburg, MD 20899	-135
1509 University Ave.	rng	Dr. Martin J. Blackburn	325
Madison, WI 53706		Pratt & Whitney  Materials Engin. Mail Stop 114-4	
Dr. Samuel Allen	513	400 Main Street	.5
Massachusetts Institute of Technology. 13-5056 77 Massachusetts Ave.		E. Hartford, CT 06108	
Cambridge, MA 02139		Dr. William Boettinger NIST, A153-B1dg. 223	509
Agren	623	Gaithersburg, MD 20899	
Division of Physical Metallurgy			
Royal Inst. Technology		Richard Braun	504
S-100 44 Stockholm, Sweden		Dept. of Engineering Sciences	
Dr. Iver Anderson	713	Technological Inst. Northwestern Evanston, IL 60208	Univ.
Ames Lab. & Iowa State University			202
122 Metals Development BLDG. Ames, IA 50011		Yves Brechet CR. Pechiney, 38000 Vorteppe France	302
Alan Ardell	O.C.		
University of California		Manfred Breiter	622
Dept. of Materials Science & Engine 5732-J BH Los Angeles, CA 90024-		Inst. Techn. Elektrochem 9 Getreidemarkt	
Dr. Harry Atwater	622	Wien, Austria 1060	
Caltach, MS 128-95	V 4	Dr. John Brooks	621
Pasadena, CA 91125		Sandia National Labs. 312 Livermore, CA 94550	<b>72.</b>
Dr. Michael Aziz	526		
Harvard University		William Brower Jr.	621
Division of Applied Sciences, 29 On Cambridge, MA 02138	xford St.	Marquette University Dept. of Mech. & Indust. Enginee	er.
	(22	1515 W. Wisconsin Ave.	
Dr. Hans Bakker University of Amsterdam	623	Milwaukee, WI 53233	
Valckenierstr. 65		Dr. Robert Brown	324
Amsterdam, The Netherlands NL1018X		Massachusetts Institute of Techr Chemical Engineering Dept. 66-34	
Dr. Srikumar Banerjee	326	Cambridge, MA 02139	
Bahadha Atomic Research Center Metallurgy Div. Bombay, India 400	085		

Dr. Lucien Brush University of Washington Dept. of Materials Sci. & Engin. 325 Robers Hall FB-10 Seattle, WA 98195	323	Dr. James Dela'O Michigan Technological University Metallurgical Materials Eng. Dept Houghton, MI 49931	
Dr. Benjamin Burton NIST, Al53/223 Gaithersburg, MD 20899	519	Larry DeVries MEB 2000 University of Utah Salt Lake City, Utah 84112	o.c.
Dr. Daniel Butrymowicz National Institutes of Standards & Materials Bldg., RM B309 Materials Science & Engineering Lab Gaithersburg, MD 20899		Dr. James Early National Institutes Of Standards Materials Bldg., Rm B309 Materials Science & Engineering I Gaithersburg, MD 20899	220 Lab.
Dr. John Cahn NIST, 223/A153 Gaithersburg, MD 20899	222	Dr. John Elmer Lawrence Livermore National Lab. PO Box 808, L355 Livermore, CA 94551	617
Dr. Ray Carpenter Center for Solid State Science Arizona State University Tempe, Arizona 85287-1704	405	Dr. Paul Evans Alcan International Banbury Lab., Southam Rd. Banbury, Oxon, England OX 16 752	219
Dr. William Cassada III Reynolds Metals Company Corporate Research & Development 4th & Canal St. Richmond, VA 23229	717	Dr. Harold Frost Dartmouth College Thayer School of Engineering Hanover, NH 03755	611
Dr. Long-Qing Chen Rutgers University Dept.of Matl. Sci., PO Box 909 Piscataway, NJ 08855-0909	620	Pro. Hans Fecht University of Augsburg Inst. of Physics Memmingerstr. 6 8900 Augsburg Germany	721
Dr. Jerome Cohen Northwestern University McCormick School of Engineering Evanston, IL 60208	619	Dr. Steven Fishman Office of Naval Research 800 N. Quincy St. Arlington, VA 22217	217
Dr. Ulrich Dahmen National Ctr. for Electron Microsco Lawrence Berkeley Lab, BLDG. 72 1 Cyclotron Rd. Berkeley, CA 94720	221 PPY	Peter Frankwicz University of Wisconsin Dept. of Materials Sci. & Engin. 1509 University Ave. Madison, WI 53706	511
Or. Jonathan Dantzig University of Illinois Dept.of Mechanical & Industrial Eng 1206 West Green St.	619	Dr. Frank Gayle NIST, RM 223/A153 Gaithersburg, MD 20899	519
Orbana, IL 61301  Or. Siddhartha Das University of WIsconsin-Madison Dept. of Materials, Science & Eng. 1509 University Ave. fadison, WI 53706	507	Dr. Uwe Glatzel Stanford University Dept. of Materials Science & Eng TU-Berlin, BH18,7000 Berlin 12 F Stanford, CA 94305-2205	

Dr. Rolf Gotthardt Ecole Polytechnique Federale Lausan Lausanne, Switzerland CH-1015	406 ine	Dr. Bimal Kad Ohio State University 116 W. 19th Ave. Columbus OH 43210	607
Dr. Douglas Granger	407		
Alcoa Lab., Alcoa Technicla Center Alcoa Center, PA 15069		Mike Kaufman University of Florida 201 Rhines Hall	502
Dr. A Greer University of Cambridge	211	Dept. of Materials Science & Eng Gainesville, FL 32611	r.
Dept. of Materials Science & Metall Pembrooke St. Cambridge, UK CB2 2QZ		Pro. Ryoichi Kikuchi University of California, Los An Materials Science & Engineering	408 geles
Dr. Amitava Guha Brush Wellman Inc. 17876 St. Clair Ave.	209	Los Angeles, CA 90024-1595  Dr. Carl Koch	321
Cleveland, OH 44110  Dr. Carol Handwerker	o.c.	North Carolina State University Materials Science & Eng. Depc. PO Box 7907	341
NIST, 233/A153 Gaithersburg, MD 20899	0.0.	Raleigh, NC 27695	
Dr.Stewart Harris SUNY, CEAS	611	Dr. David Lee USAF, Materials Directorate, WL/ WPAFB, OH 45433	411 MLLM
Stony Brook, NY 11794		David Y. Lee	618
David Hoglund Harvard University Gordon Mskay L3 9 Oxford Street Cambridge, MA 02138	608	Materials Sci. & Engin. Postech Pohang, Korea 790-600	
Dr. William Hopfe	608	Richard Lewis LMSC Inc., 93-10/204	502
University of Connecticut Box U-136, Dept. of Metallurgy Storrs, CT 06269-3136		3251 Hanover St. Pal Alto, CA 94304	
Dr. James Howe University of Virginia	208	Dr. Harry Lipsitt Wright State University Dept. of Mech. & Mats. Eng.	420
Dept. of Materials Science, Thornto Charlottesville, VA 22902-2442	on Hall	Dayton, OH 45435	
Dr. J D Hunt University of Oxford Dept. of Materials, Parks Rd.	O.C.	Dr. A Loiseau ONERA, 29 Ave. DE LA Division La BP 72 Chatillon France 92322	320 clerc
Oxford, United Kingdon OX1 3PH		Dr. Blair London Howmet Corp. 1500 S. Warner St.	409
Dr. Gerhard Inden Max-Planck-Institut Eisenforschung Max-Planck-Str. 1	206	Whitehall, MI 49461-1895  Dr. David Luzzi	426
Dusseldord Germany  Dr. Mel Jackson	205	University of Pennsylvania Dept. of Materials Science 3231 Walnut St.	
General Electric CRD, K-1 MB 223 Bo Schenectady, WY 12301	<del>-</del>	Philadelphia, PA 19104-6272  Dr. Steven Marsh	607
Dr. William Johnson Carnegie Mellon University 3325 Wean Hall Pittsburgh, PA 15213-3890	505	Naval Research Lab. Code 6325 Washington, DC 20375-5000	uu r

Dr. Patrick Martin	319	Dr. Tai Nguyen	605
Rockwell International Science Cent		L3L/UC Berkeley	
1049 Camino Dos Rios		Lawrence Berkeley Lab.	
		MS 2-400, 1 Cyclotron Rd.	
Thousand Oaks, CA 91360		Berkeley, CA 94720	
	/:0	berketey, CA 94710	
Dr. Carolyn MacDonald	418	Dec Brown Oliveran	135
SUNY Albany, Physics Dept.		Dr. Ben Oliver	605
Albany, NY 12222		University of Tennessee	
		Dept. of Materials Science & Eng	
Dr. Bruce MacDonald	225	RM 425, Dougherty Engineering 31	dg.
National Science Foundation		Knoxville, TN 37996-2200	
Div. of Material Research 6800 G. S	t.		
Washington, DC 20550		Dr. David Oxtaby	317
"ao", 20", 20" - 222 - 2		University of Sydney	
Dr. Arthur McEvily	313	Dept. of Theoretical Chemistry	
University of Connecticut	5-0	Sydney, Australia NSW 2006	
		by didy, indeparted size 2009	
Masallurgy Dept., U-136		Dr. John Boronagko	509
Storms, CT 06268		Dr. John Perepezko	J ( )
		University of Wisconsin	
Dr. CJ McMahon Jr.	425	Dept. of Mat. Sci. & Eng.	
University of Pennsylvania		1509 Univ. Ave.	
Dept. of MSE, 3231 Walnut St.		Madison, WI 53706	
Philadelphia, PA 19104			
		Kevin Peters	521
Dr. Mark McCormack	625	Dept. of Materials Science	
Lawrence Berkeley Lab/UCB		Evanston, IL 60202	
· · · · · · · · · · · · · · · · · · ·			
#1 Cyclotron Rd. MS 66-200		Dr. Jean Philibert	311
Center For Advance Material/MS&ME		Universite Paris -SUD	J
Berkeley, CA 94720			
	4.10	Metallurgie - BAT 413	
Dr. Jyothi Menon	410	Orsay France F-91405	
Wright Patterson Air Force Base			( ) )
WI/MIM		Dr. David Pope	603
Wright-Patterson A, OH 45433-6533		University of Pennsylvania	
-		MEAM Dept. Towne Bldg.	
Dr. John Morral	606	220 S. 33rd St.	
University of Connecticut		Philadelphia, PA 19104-6315	
97 N. Eagleville Rd., RM 111			
Storrs, CT 06269-3136		Dr. Gary Purdy	424
505223, 61 0020) 5130		McMaster University 1280 Main St	. West
Dr. James Morris	606	Materials Science & Engineering	
	300	Hamilton, Ontario, Canada L8S 41	.7
University of Kentucky		namifically officially said and a	- •
Light Materials Research Labs.		Dr. James Rawers	310
Anderson Hall			J 2 G
Lexington, KY 40506		US Bureau of Mines	
		Albany Research Center	
Dr. John Morris Jr.	625	1450 SW Queens Ave.	
University of California, Berkeley		Albany, Oregon 97333	
One Cyclotron Rd. MS 66-800			
Manter for Advance Materials/MS&ME		Steven H. Reichman	309
Berkeley, CA 94720		Wyman-Gordon, Worcester St.	
		North Grafton, MA 015	
Dr. Donokuu No	521	.•	
Dr. Dongkyu Na	J ~ -	Dr. Rosenberg	308
Northwestern University	ain	IBM TJ Watson Research Center	
Tech. Inst. of Materials Sci. & En	5	PO Box 210	
2145 Sheridan			
Evanston, IL 60201		Yorktown Heights, NY 10598	

Dr. Alan Rosenstein A.F.O.S.R., AFOSR/NE Bldg. 410 Bolling AFB Washington, DC 20332	306	Dr. Seiji Takeda Osaka University College of General Education Toyonaka, Csaka Japan 560	624
Dr. Alexander Roytburd University of Maryland Materials & Nuclear Engineer. Dept College Park, MD 20742-2115		Dr. Lee Tanner Lawrence Livermore Nat. Lab. Chemistry & Materials Science 7000 East Ave. Livermore CA 94550	402
Dr. Vladimir Segal Mechanical Engineering University of Delaware Newark, DE 19716	525	Dr. Nagappan Thangaraj National Center for Electron Mic Bldg. 72 Lawrence Berkeley Lab 1 Cyclotron Rd.	226 roscopy
Dr. Adam Schwartz Lawrence Livermore NL L-355 PO Box	303 808	Berkeley, CA 94720	
Dr. Yoontto Son University of Connecticut Dept.of Metallurgy, U-136 Storrs, CT 06268	602	Dr. Dan Thoma University of Wisconsin-Madison Dept. of Materials Science & Eng 1509 University Ave. Madison, WI 53706	507 in.
Dr. David Skinner Allied Signal Research & Technolog PO Box 1021, Columbia Rd. Morristown, NJ 07962	602 y	Dr. Anthony Thompson Carnegie Mellon University Dept. of Metallurgy & Engin. Pittsburgh, PA 15213	604
Dr. Frans Spaepen Harvard University Division of Applied Sciences	722	Dr. Ariel Traiber M.I.T. Rm 13-5126 Cambridge, MA 02139	604
29 Oxford Street Cambridge, MA 02138		Dr. Rohit Trivedi Iowa State University 100 Wilhelm Hall	524
Dr. Brian Spencer Northwestern University Dept. ES/AM Technological Inst. Evanston, IL 60208	504	Ames, IA 50011  Dr. David Van Aken University of Michigan	508
Dr. James Staley ALCOA, ALCOA Labs ALCOA Tech. Center, PA 15069	422	2300 Hayward St. Dept.Mater Sci. & Engineering Ann Arbor, MI 48109-2136	
Dr. James Steele Jr. Los Alamos National Lab Mail Stop E506 Los Alamos, NM 87545	522	Dr. Roy Vandermeer Naval Research Lab, Code 6320.1 4555 Overllok Ave. Washington, DC 20375-5000	419
Dr. P R Subramanian Universal Energy Systems Inc. Materials Research Division 4401 Dayton-Xenia Road	610	Dr. Frans Van Loo Eindhoven University of Technolo Lab. TVM-CTK, PO Box 513, 5600 MB Eindhoven The Netherlan	ıds
Dayton, OH 45432  Dr. Bruce Taggart	624	Dr. Clinton Van Siclen EG&G Idaho, Inc. Inel Research Center, Phys. & Ma	223 it. Group
National Science Foundation Division of Materials Research 1800 G.St. NW Washington, DC 205		PO Box 1625 Idaho Falls, ID 83415-2211	·

Dr. Vijay Vasudevan University of Cincinnati Dept. of Materials Science & Engine ML 12 Cincinnati, OH 45221	524 ering
Dr. Peter W. Voorhees Northwestern University Dept. Materials Science & Engineeri Evanston, IL 60208	505 .ng
Dr. David Vul University of California, Berkeley Dept. of Materials Science & Minera Berkeley, CA 94720	
Dr. John Wei RES-12 Timken Co. 1335 Dueber Ave. S.W. Canton, OH 44706	202
Or. GErhard Welsch Case Western Reserve University 10900 Euclid Ave. Cleveland, OH 44106	523
Zhang Wenzheng McMaster University Dept. of Materials Sci & Engineerin 1230 Main St. W. Hamilton, Ontario, Canada 285 4L7	403 1g
Dr. A A Wheeler NIST, C/O Robin Bickel AISI Technology NIST Caithersburg, MD 20899	510
Dr.George Yoder Office of Naval Research Materials Division, Code 1131 800N. Quincy St. Arlington, VA 22217-5000	204
Or. Frederick Yost Sandia National Lab. Dept. 1830A Albuquerque, NM 87108	203
Dr. Jacob Zindel Ford Motor Company Rm S-2046 SRL PO Box 2053 Dearborn, MI 48121-2053	508

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